Electronic Supplementary Material (ESI) for Nanoscale.

Functionalized MXenes as Effective Polyselenides Immobilizer for Lithium-Selenium Batteries: A Density Functional Theory (DFT) Study

Rahul Jayan, Md Mahbubul Islam*

Department of Mechanical Engineering, Wayne State University, Detroit, MI 48202, USA

*Corresponding author: mahbub.islam@wayne.edu

Table S1. Structural data of the bare and functionalized Mxenes

AM	Lattice Parameters (A°)		Bond length (A°)	
	a = b	Ti - C	Ti - Ti	Ti – S/O/F/Cl
Ti_3C_2	12.370	2.05	2.92	-
$Ti_3C_2S_2$	12.493	2.16	3.03	2.40
$Ti_3C_2O_2$	12.108	2.18	3.10	1.97
$Ti_3C_2F_2$	12.215	2.06	2.94	2.16
$Ti_3C_2Cl_2$	12.108	2.05	2.93	2.47

Table S2. The binding energies (in eV) of higher order polyselenides with the electrolyte solvents

Higher order Li_2Se_n polyselenides	DME	DOL
Li_2Se_4	0.87	0.82
Li_2Se_6	0.92	0.79
Li_2Se_8	0.90	0.83

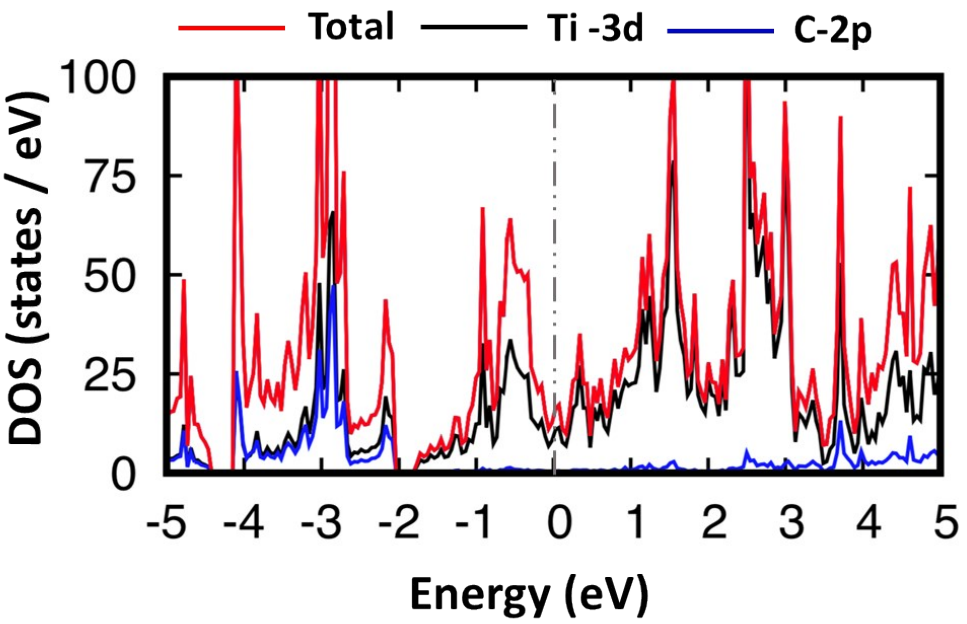

Fig S1. Partial density of states (PDOS) of Ti_3C_2. The fermi level is indicated with a vertical line

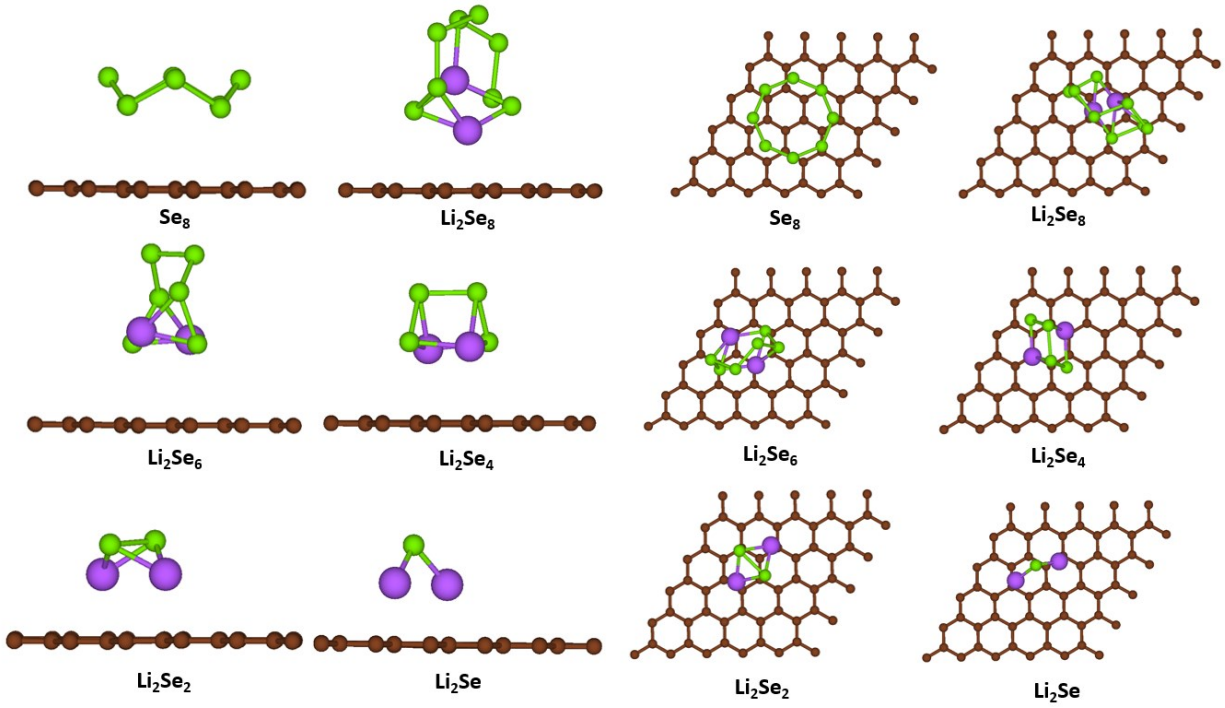

Figure S2. Top and side views of the structures of Li_2Se_n adsorbed monolayer graphene

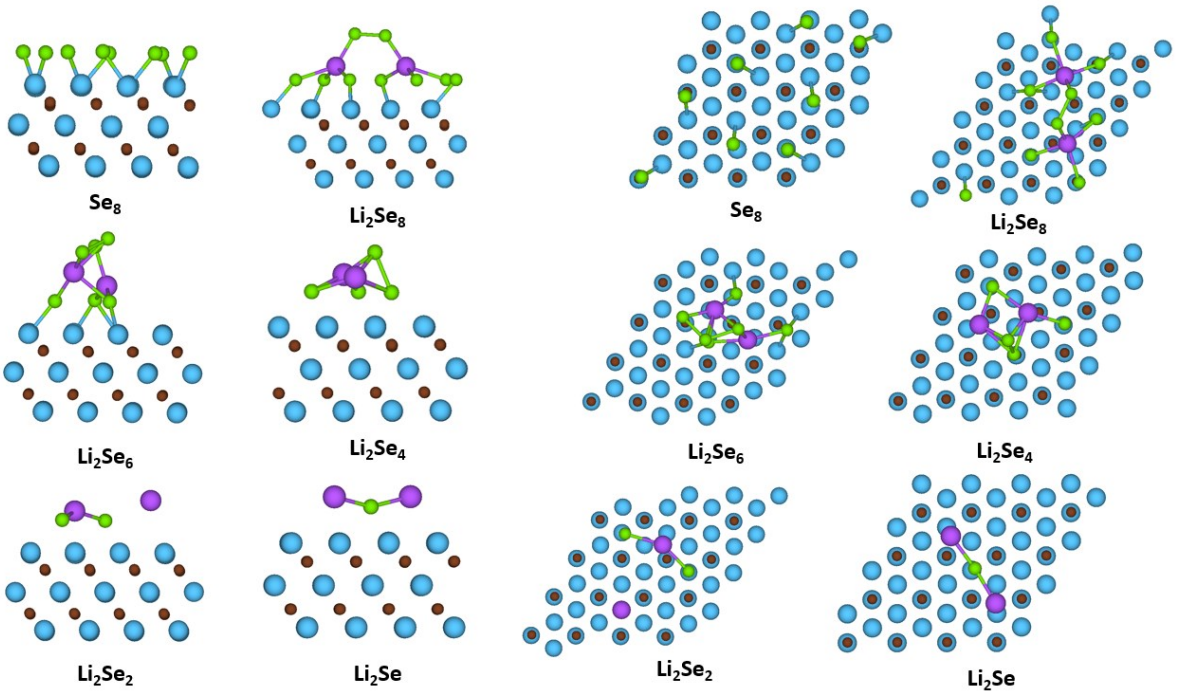

Figure S3. The side and top views of the most stable structures of Li_2Se_n adsorbed on Ti_3C_2

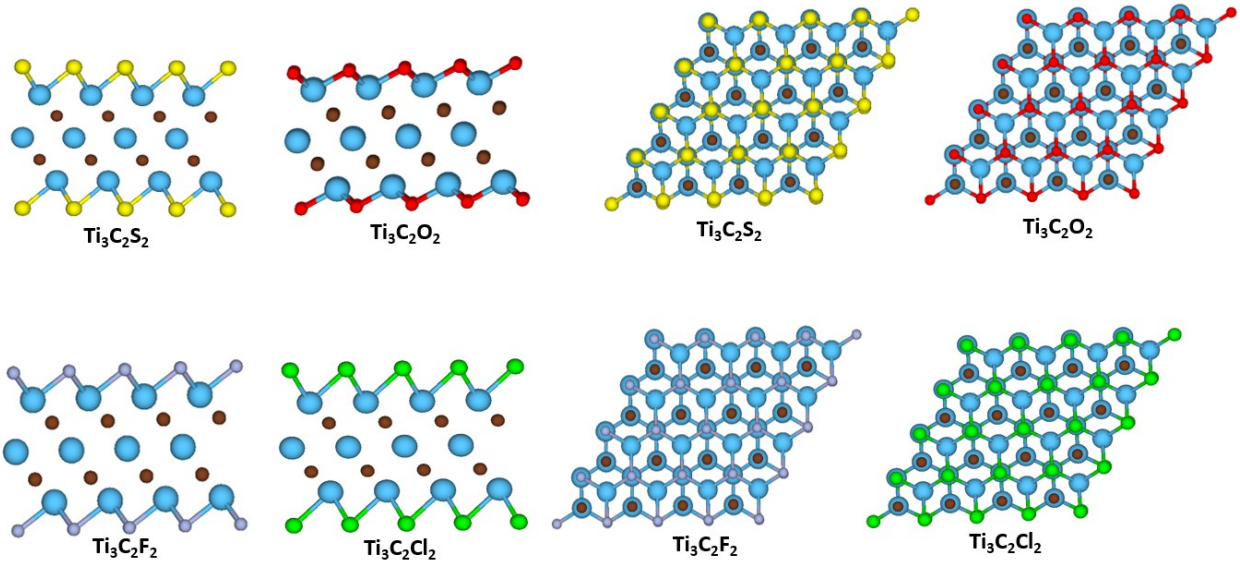

Figure S4. The side and top views of the optimized structures of $Ti_3C_2X_2$ (X = S, O, F, Cl)

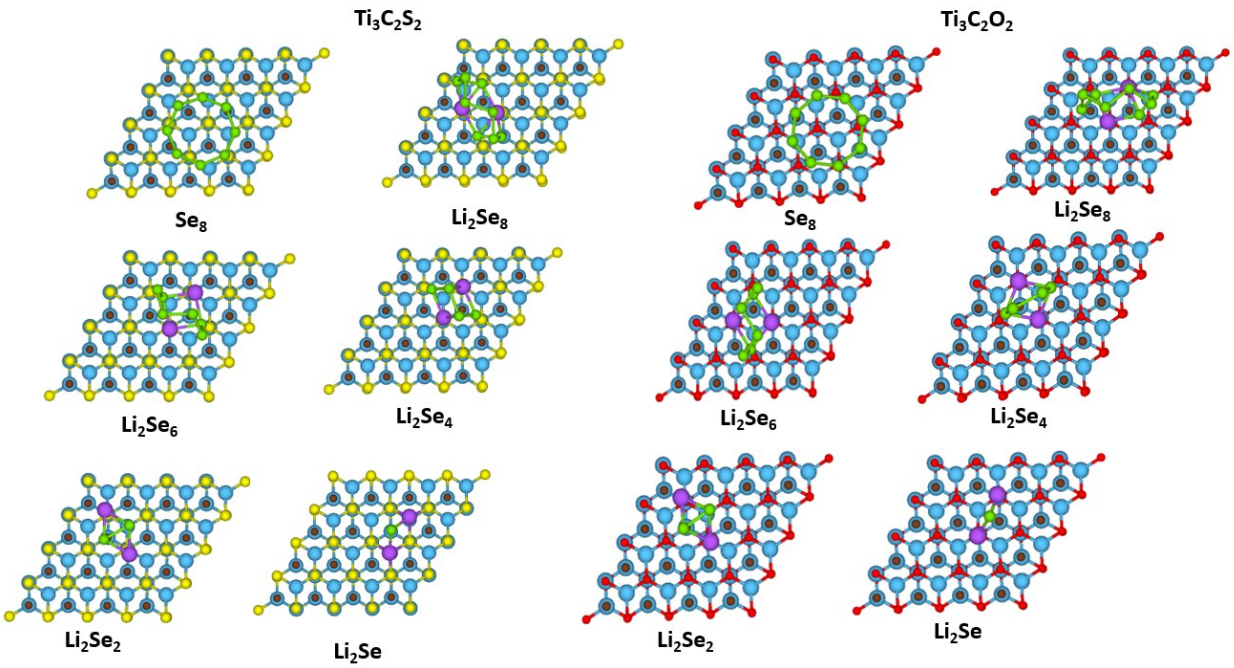

Figure S5. The top views of the most stable structures of Li_2Se_n adsorbed on $Ti_3C_2S_2$ and $Ti_3C_2O_2$.

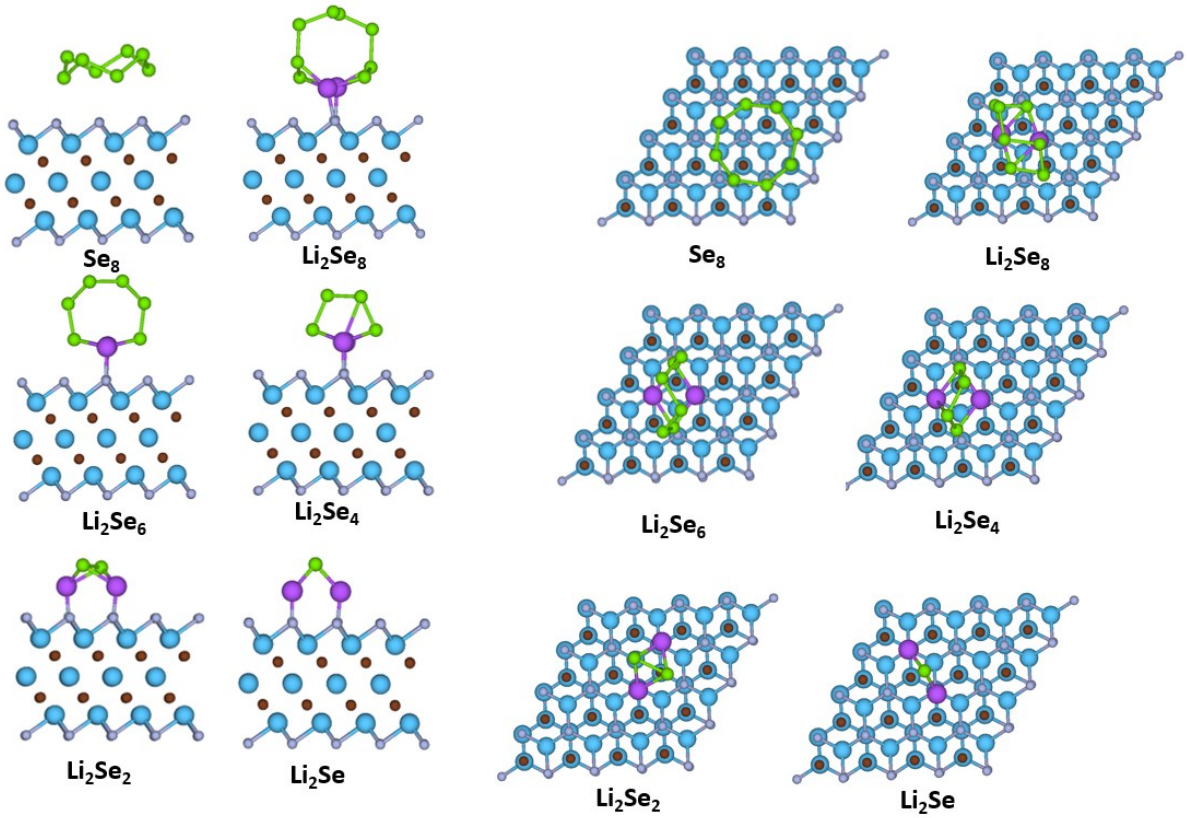

Figure S6. The side and top views of the optimized structures of Li_2Se_n adsorbed $Ti_3C_2F_2$

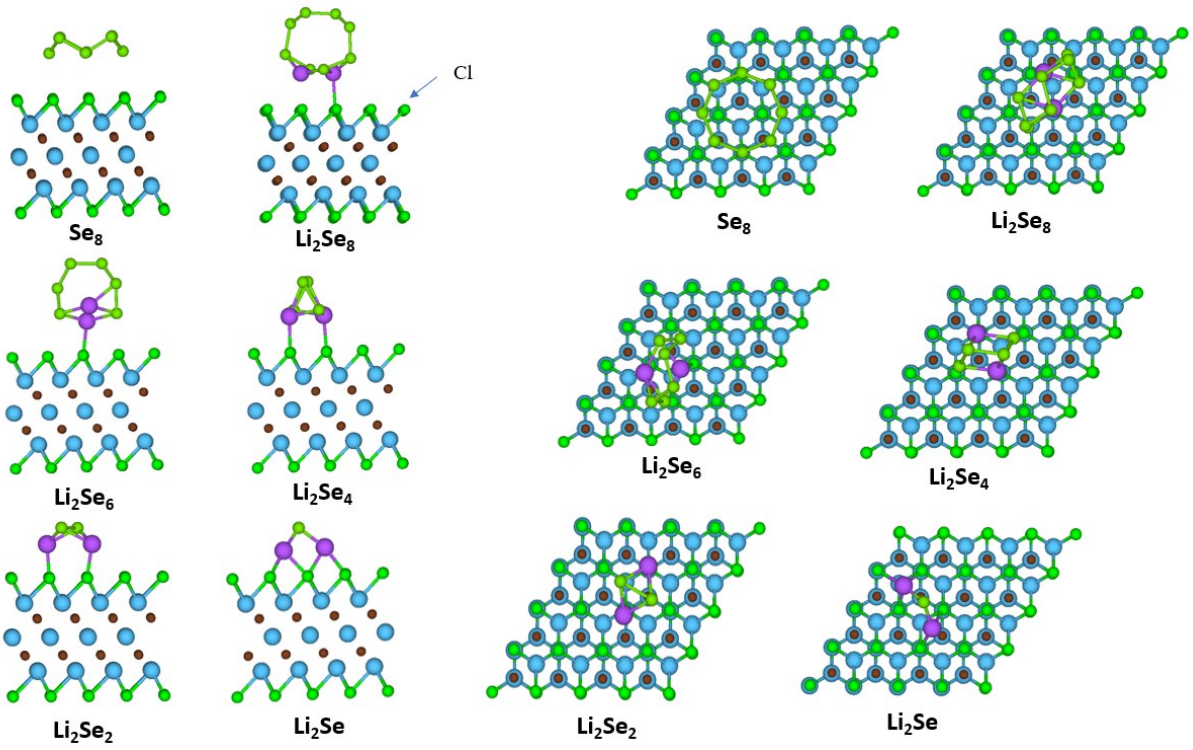

Figure S7. The side and top views of the most favorable configurations of Li_2Se_n adsorbed $Ti_3C_2Cl_2$

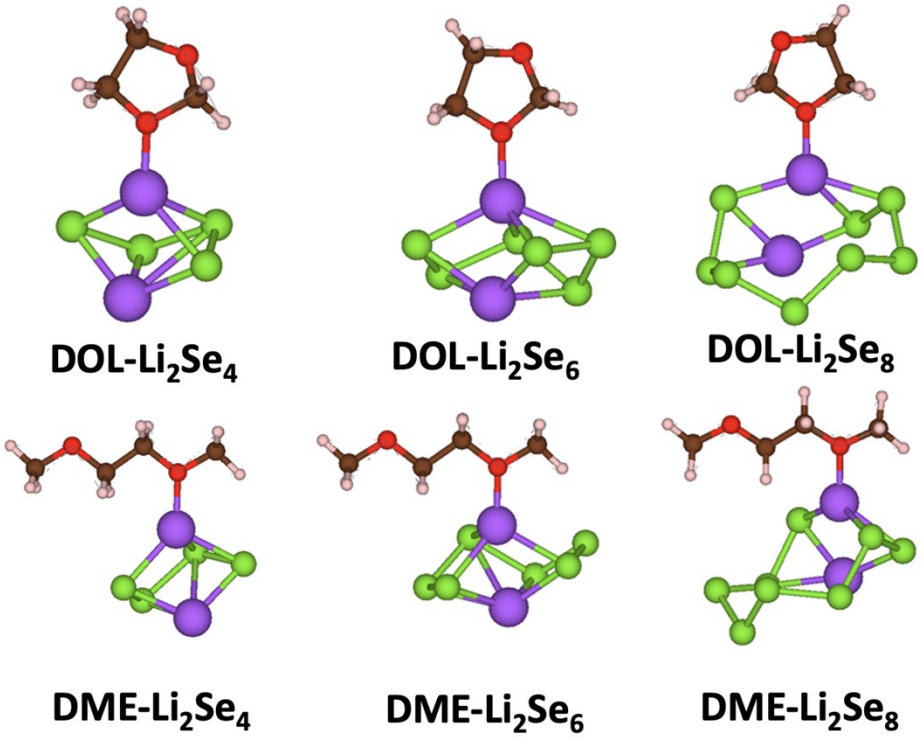

Figure S8. The most stable geometric configurations of ($Li_2Se_n \geq 4$) bound DOL/ DME solvents

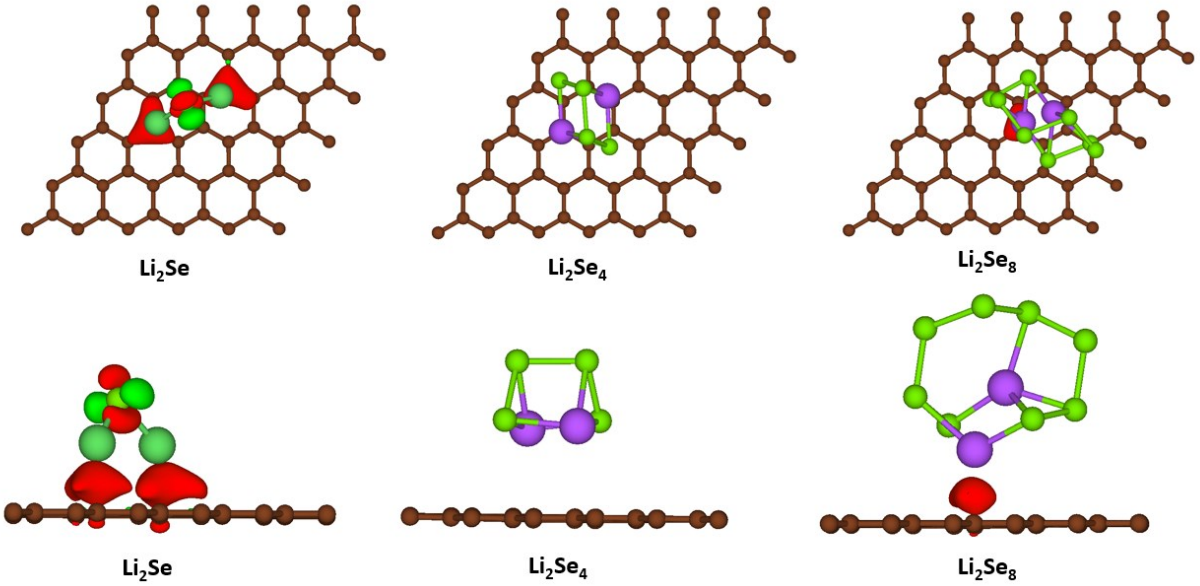

Figure S9. Charge density difference of Li_2Se_n (n = 1,4,8) on graphene. The iso-surface level is set at 0.0020 e $Å^{-3}$. The green and red colors denote charge accumulation and depletion, respectively.

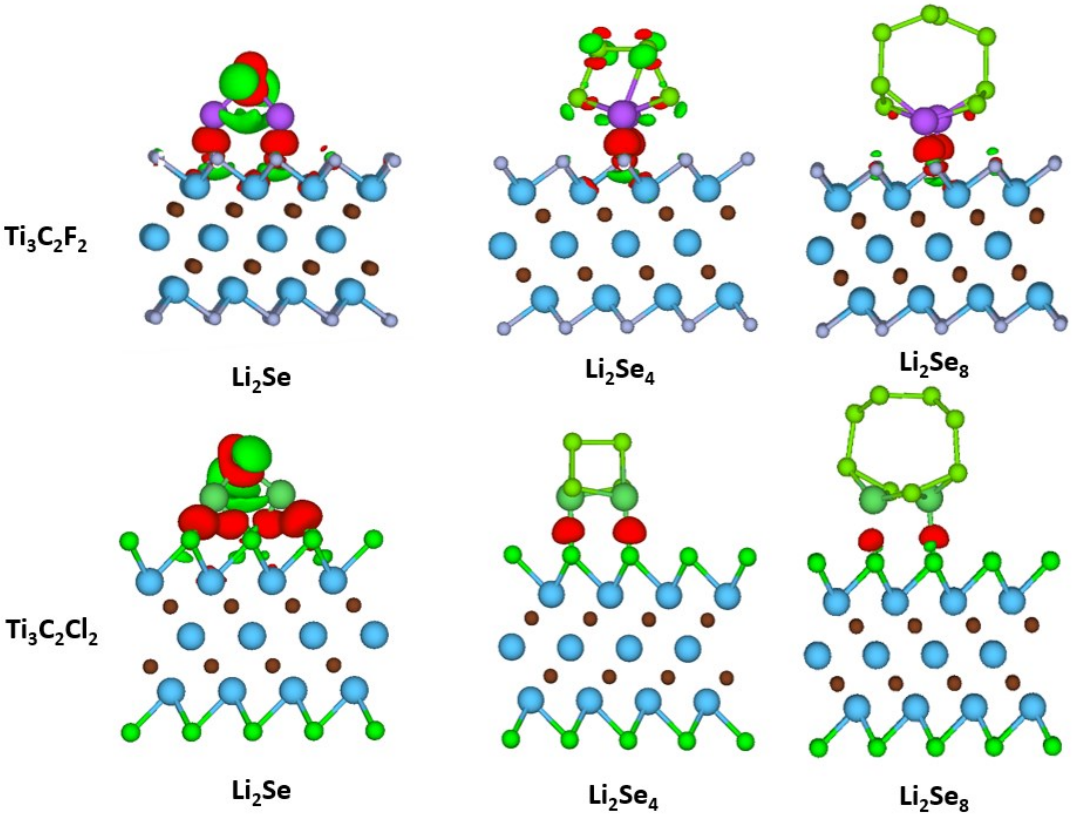

Figure S10. Charge density difference of Li_2Se_n (n = 1,4,8) on $Ti_3C_2F_2$ and $Ti_3C_2Cl_2$. The iso-surface level is set at 0.0020 e $Å^{-3}$. The green and red colors denote charge accumulation and depletion, respectively.

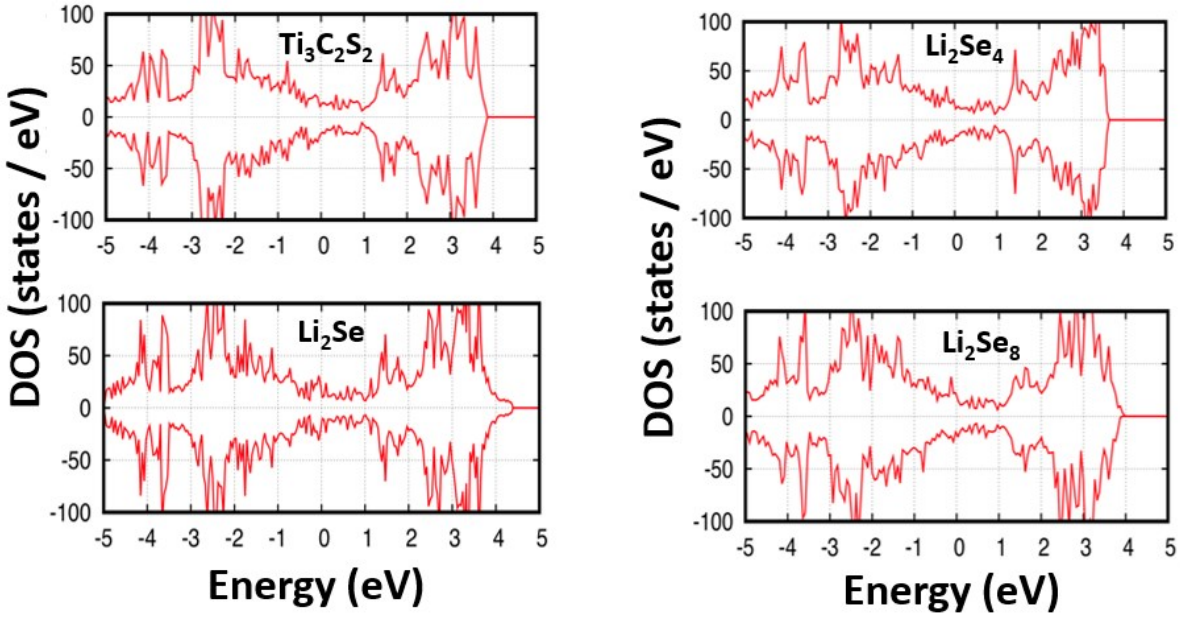

Figure S11. Total DOS of Li_2Se_n (n = 1,4,8) adsorbed $Ti_3C_2S_2$.

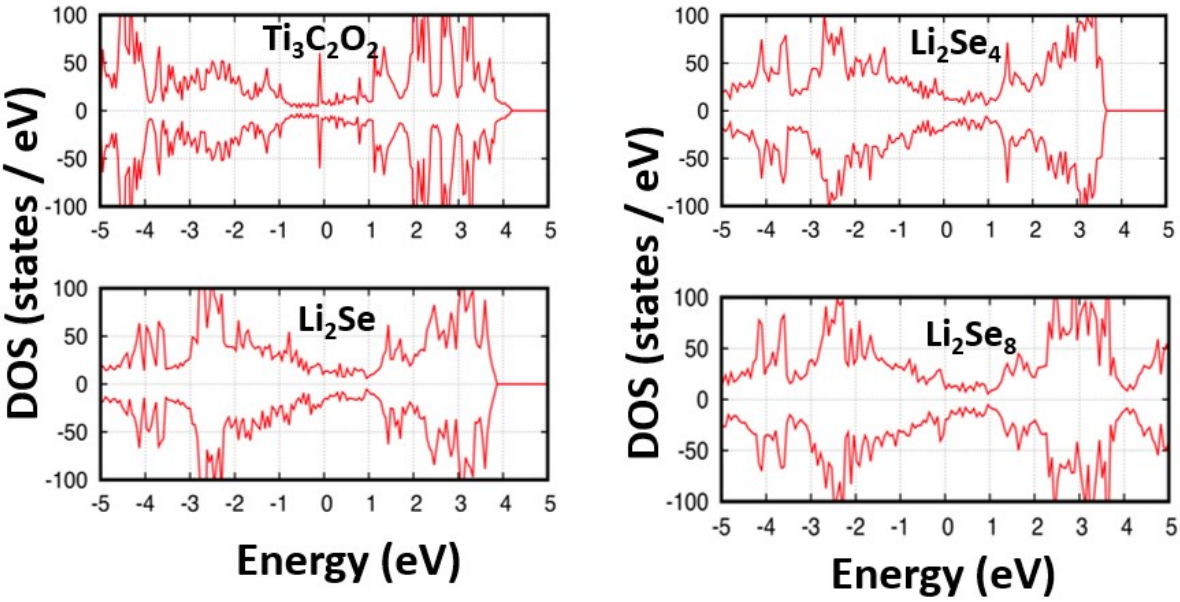

Figure S12. Total DOS of Li_2Se_n (n = 1,4,8) adsorbed $Ti_3C_2O_2$

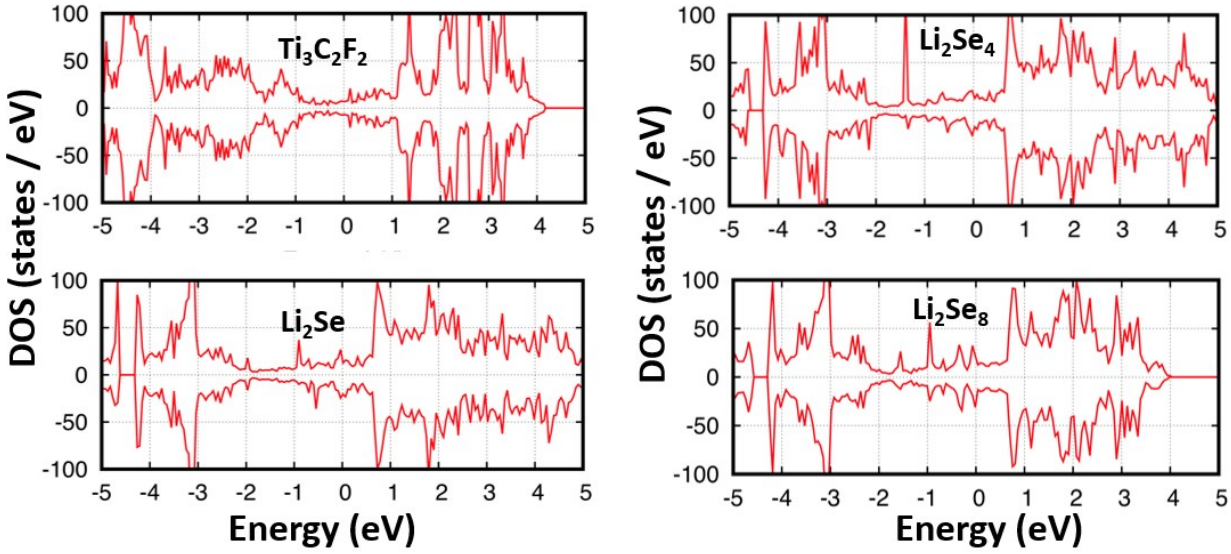

Figure S13. Total DOS of Li_2Se_n (n = 1,4,8) adsorbed $Ti_3C_2F_2$

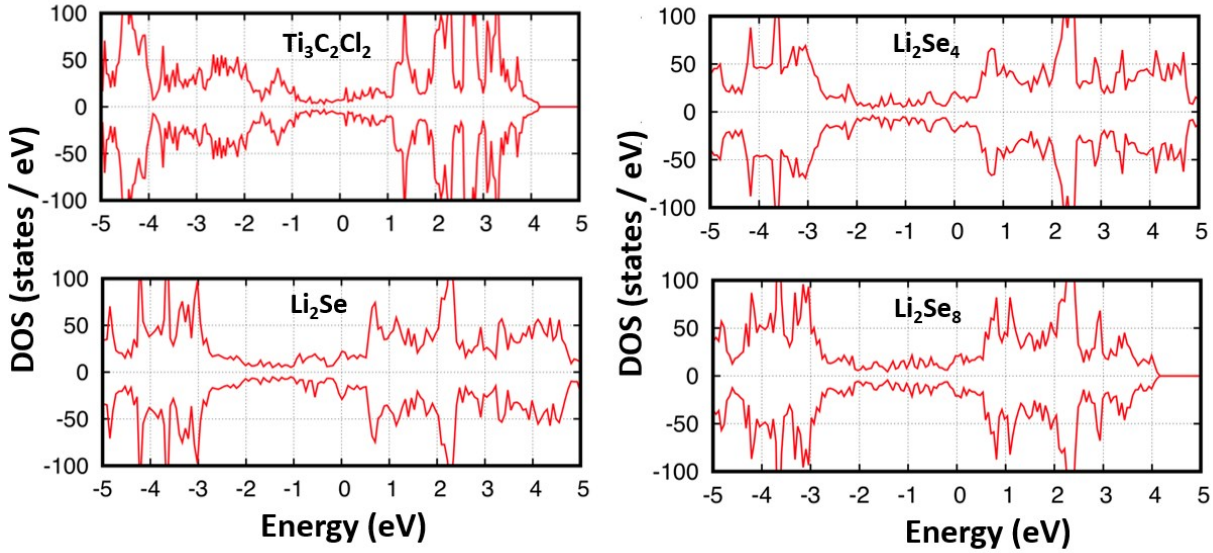

Figure S14. Total DOS of Li_2Se_n (n = 1,4,8) adsorbed $Ti_3C_2Cl_2$

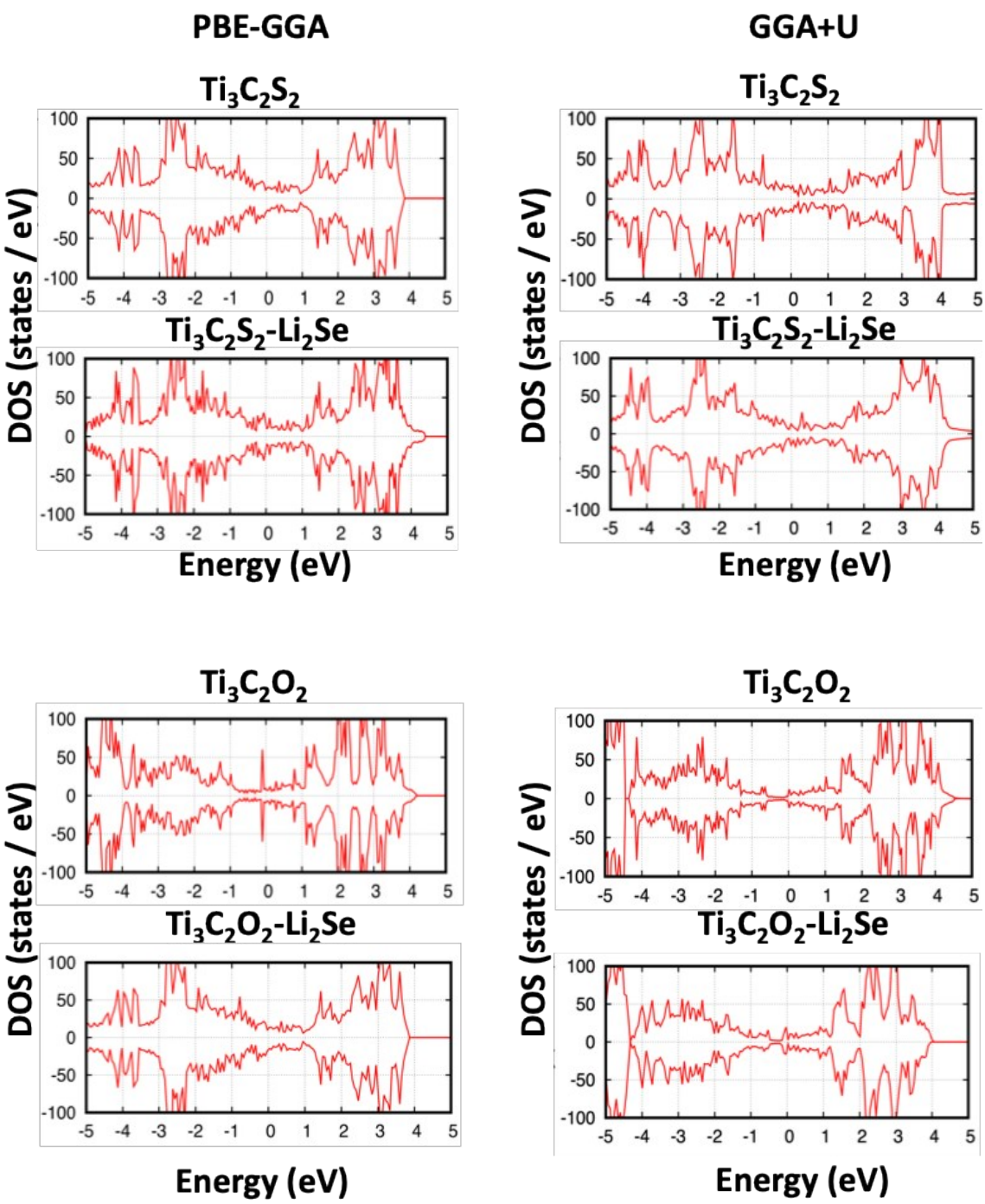

Figure S15. Total DOS of Ti_3C_2-S/O and Ti_3C_2-S/O-Li_2Se calculated using PBE-GGA and GGA+U method